



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 04:15 PM EDT

PDB ID : 1FRV
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on : 1996-03-28
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

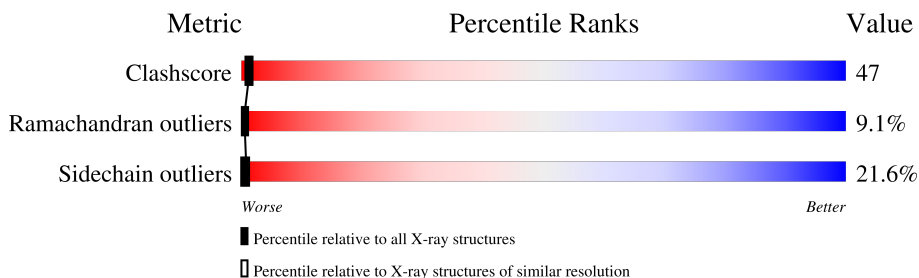
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	C	264	
2	B	536	
2	D	536	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	C	265	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12268 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

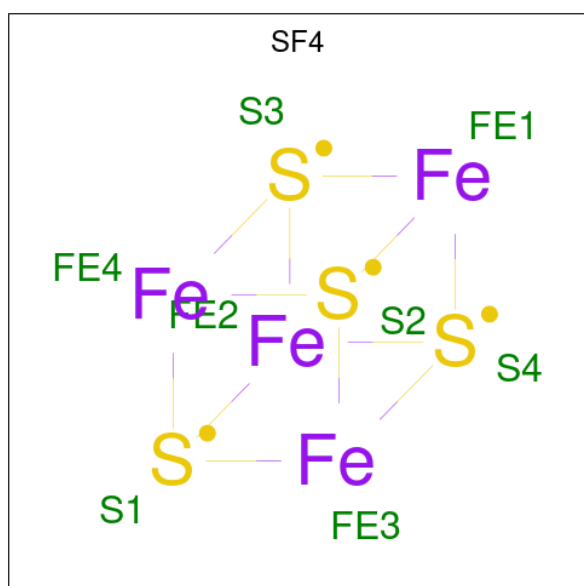
- Molecule 1 is a protein called HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			
1	C	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			

- Molecule 2 is a protein called HYDROGENASE.

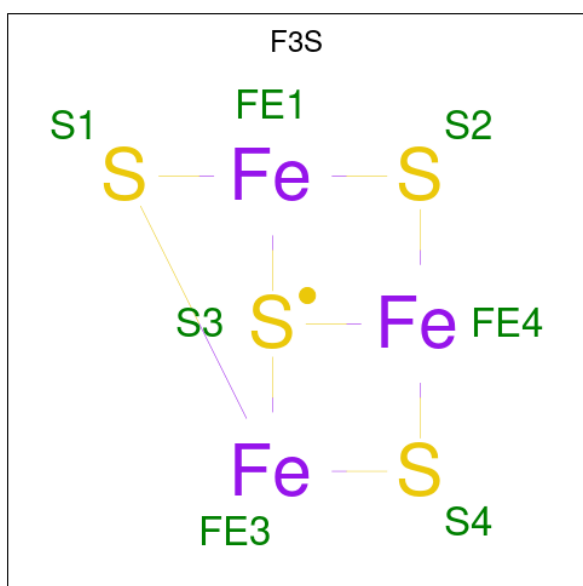
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			
2	D	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

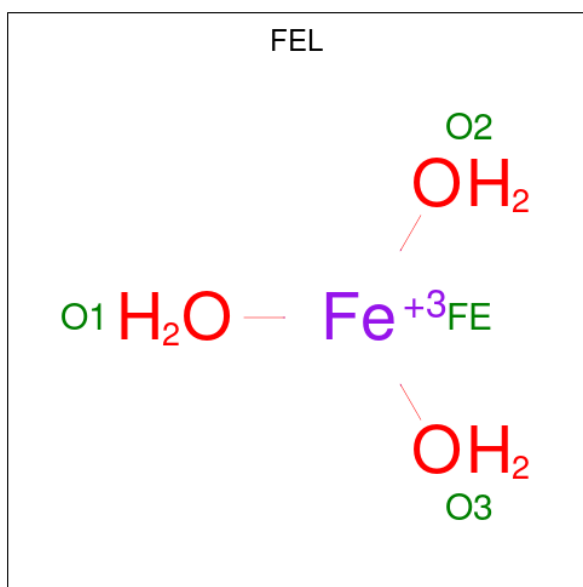


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		

- Molecule 6 is HYDRATED FE (three-letter code: FEL) (formula: FeH_6O_3).



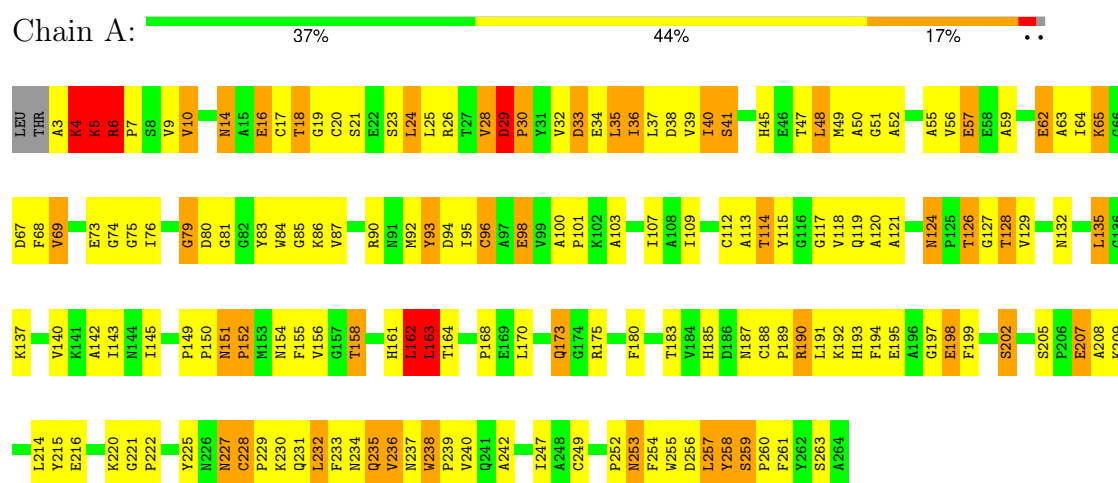
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	O	0	0
			4	1	3		
6	D	1	Total	Fe	O	0	0
			4	1	3		

3 Residue-property plots

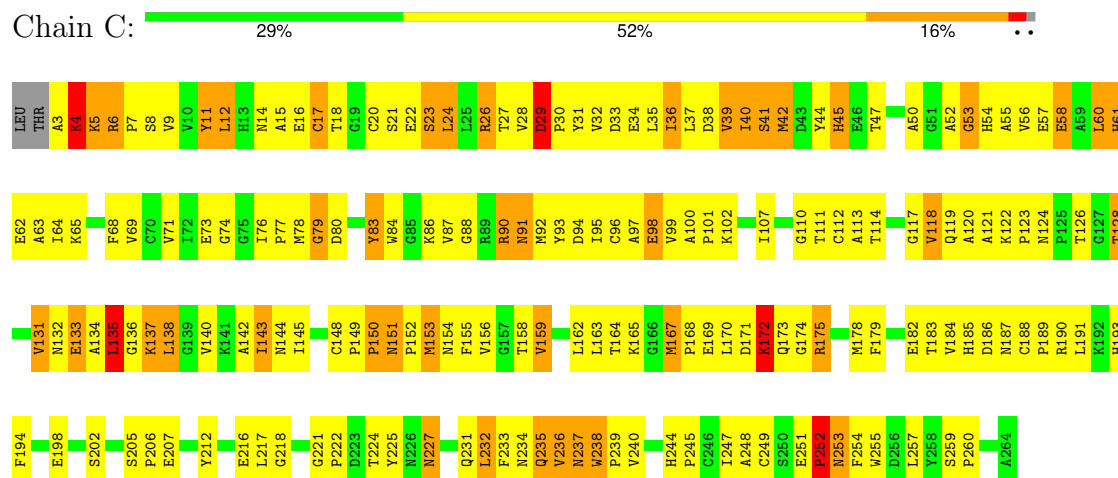
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: HYDROGENASE



• Molecule 1: HYDROGENASE



• Molecule 2: HYDROGENASE



MET	G66	P131	E198	K289	P343	L404	Q472	P343	K289	E198	P131	G66	MET
SER	V67	A132	A199	N270	K344	F405	R473	K344	N270	A199	A132	V67	SER
GLU	C68	K133	L200	W271	W345	S406	G474	W345	W271	L200	K133	C68	GLU
MET	T69	A134	R201	A272	T346	T407	G475	T346	A272	R201	A134	T69	MET
GLN	C68	G273	L408	K476	E347	G409	K477	E347	K476	L408	G273	C68	GLN
GLY	V71	Y70	Q203	I274	F348	R410	I477	F348	I274	Q203	Y70	V71	GLY
K7	H72	L137	G203	T277	H349	R411	E478	H349	T277	G203	L137	H72	K7
K8	A73	A138	A211	S278	G350	T411	R479	G350	S278	A211	A138	A73	K8
I9	L74	N139	I212	S278	E351	A412	F490	E351	S278	I212	N139	L74	I9
V10	A75	D140	F213	N279	D352	R413	Q481	D352	N279	F213	D140	A75	V10
V11	S76	L141	G214	F280	R353	R414	H482	R353	F280	G214	L141	S76	V11
I14	V77	S142	G216	T282	G354	G415	V483	G354	T282	G216	S142	V77	I14
T15	A78	R143	N217	C283	S355	I416	V484	S355	C283	N217	R143	A78	T15
R16	V80	K145	P218	C283	W356	Q417	P485	W356	C283	P218	K145	V80	R16
R17	V80	T146	H219	T288	R357	C418	S486	R357	T288	H219	T146	V80	R17
E18	N82	T147	T220	D289	K358	L419	T487	K358	D289	T220	T147	N82	E18
G19	C83	T148	Q221	P360	A359	T420	L490	A359	P360	Q221	T148	C83	G19
H20	V84	E149	R222	D292	R361	A421	G491	R361	D292	R222	E149	V84	H20
R21	G85	S150	T223	L293	Y362	E424	P492	Y362	L293	T223	S150	G85	R21
R22	V86	L151	T224	K363	R362	V425	P492	R362	K363	T224	L151	V86	R22
I23	K87	A152	V225	S295	G364	W428	C494	G364	S295	V225	A152	K87	I23
E24	I88	A153	G226	E365	E365	W428	A495	E365	G226	E24	A153	I88	E24
V25	P89	V154	G227	A366	F367	D429	E496	F367	V154	G227	V154	P89	V25
E26	E90	G155	C228	G300	E366	D430	R497	E366	G300	C228	G155	E90	E26
V27	N91	A156	T229	V302	E368	K431	K488	E368	V302	T229	A156	N91	V27
E28	A92	A157	N230	I303	V369	L432	L499	V369	I303	N230	A157	A92	E28
G29	T93	V158	G231	W304	E433	A433	S500	E433	W304	G231	V158	T93	G29
G30	L94	K159	D232	G306	P371	A434	A501	P371	G306	D232	K159	L94	G30
K31	N95	A160	S233	N305	L372	N435	V502	L372	N305	S233	A160	N95	K31
I32	R96	A160	L234	D307	A373	V436	E503	A373	D307	L234	A160	R96	I32
K33	R97	E163	L239	L308	S374	K437	Q504	S374	L308	L239	E163	R97	K33
R34	L98	S164	A240	V311	V375	A438	T509	V375	V311	A240	S164	L98	R34
A35	M100	Q166	E241	D312	L376	Q439	P510	L376	D312	E241	Q166	M100	A35
W36	T99	Q166	A241	D312	V377	K440	P510	V377	A241	A241	T99	W36	W36
S37	Q103	L167	F242	P316	A378	D441	I511	A378	P316	F242	L167	Q103	S37
M38	Y104	I169	R243	D317	Y379	L443	D513	Y379	D317	R243	I169	Y104	M38
S39	Y105	F170	K244	L318	A380	L443	P514	A380	L318	K244	F170	Y105	S39
T40	H106	T171	Y246	E320	K382	Y444	R516	K382	E320	H106	T171	H106	T40
F42	D107	N172	K247	E321	H383	T445	P517	H383	E321	D107	N172	D107	F42
R43	H108	A173	E248	H322	E384	T451	V518	E384	H322	H108	A173	H108	R43
G44	L109	L110	G44	V323	P385	E452	E519	P385	V323	L109	L110	G44	G44
L45	V110	L176	F252	K324	T386	S453	E519	T386	K324	V110	L176	F252	L45
E46	H111	G177	I253	Y325	V387	Q454	L521	V387	I253	H111	G177	I253	E46
P47	F112	G178	E254	A389	K388	G456	R522	K388	F112	P47	F112	E254	P47
I48	Y113	H179	Q255	Y325	V390	V456	T523	V390	Y113	I48	Y113	Q255	I48
L49	H114	L115	V256	Y328	V390	G457	V524	V390	H114	L49	H114	V256	L49
K50	L115	L115	E329	G390	L392	V459	Y527	L392	K50	K50	L115	E329	K50
G51	R52	V183	T257	A331	L392	V459	Y527	L392	G51	G51	R52	V183	G51
R52	L118	L184	T259	A331	L392	V459	Y527	L392	R52	R52	L118	L184	R52
D53	D119	P185	D260	H335	L394	R463	D528	L394	D53	D53	D119	P185	D53
P54	N122	E187	L261	T396	K395	G464	P529	K395	P54	P54	N122	E187	P54
R55	V123	N122	L262	T396	K395	M465	P529	T396	R55	R55	V123	N122	R55
T61	L127	I191	A263	Y337	K397	L466	A532	Y337	T61	T61	L127	I191	T61
Q62	N128	H195	Z285	G399	G399	H468	H536	G399	Q62	Q62	N128	H195	Q62
R63	A129	H196	G266	V340	G400	W469	T470	G400	R63	R63	A129	H196	R63
A64	D130	L197	F267	T341	P401	V471	H536	P401	A64	A64	D130	L197	A64

● Molecule 2: HYDROGENASE

Chain D:  18% 56% 22%

MET	A64	A126	E187	F252	D317	A390	MET
SER	C65	L127	V188	I253	L318	K381	SER
GLU	G66	N128	L189	E254	E320	K382	GLU
MET	V67	A129	L190	Q255	E320	K383	MET
GLN	T69	D130	I191	V256	H322	E384	GLN
GLY	C68	G273	A192	Y257	H322	P385	GLY
K7	V70	A132	T193	I258	V323	T386	K7
K8	V71	K133	T193	I258	K324	V387	K8
I9	H72	A134	Y196	D260	G324	K388	I9
V10	A73	A135	L197	L261	G325	K389	V10
V11	L74	R136	E198	L262	W327	V390	V11
D12	V77	L137	A199	G205	Y328	D391	D12
P13	V77	A138	L200	G205	E329	L392	P13
I14	R78	N139	R201	G205	E329	V393	I14
T15	A79	D140	V202	G205	G330	V393	T15
R16	A79	D140	Q203	F257	A331	L394	R16
R17	V80	L141	Q203	F257	D332	K395	R17
E18	N82	S142	D81	K269	A333	T396	E18
G19	C83	P143	K205	N270	P336	L397	G19
H20	V84	R144	R208	W271	G336	G398	H20
L21	G85	K145	A209	I274	V340	V399	L21
R22	V86	T147	M210	G275	T341	G400	R22
I23	K87	T148	A211	K276	K342	P401	I23
E24	I88	E149	I212	T277	P343	E402	E24
V25	P89	S150	F213	S278	K344	A403	V25
E26	E90	L151	G214	N279	W345	F405	E26
V27	N91	K152	A215	F280	T346	S406	V27
E28	R97	A153	K216	T281	E347	T407	E28
G29	T93	Q154	N217	T282	F348	L408	G29
G30	L94	Q155	P218	G283	H349	A409	G30
K31	N95	A156	H219	G284	G350	R410	K31
I32	R96	K157	T220	E285	E351	T411	I32
K33	R97	V158	Q221	F286	D352	A412	K33
N34	T99	K159	P222	T287	R353	A413	N34
A35	M100	A160	L298	T288	Y354	R414	A35
W36	G101	L161	G227	D289	S355	G415	W36
S37	Y104	V162	T228	D292	W356	T416	S37
M38	M105	E163	T229	L293	K357	Q417	M38
S39	H106	S164	N230	N294	K358	Q418	S39
T40	H106	Q166	D232	S295	A359	A418	T40
F42	D107	L167	S233	R296	P360	A421	F42
R43	H108	G168	L234	Y297	Y362	E424	R43
L48	L109	T169	R235	T298	K363	W426	L48
L49	V110	F170	P236	P299	G364	E426	L49
K50	H111	T171	E237	Q300	E365	V427	K50
G51	F112	N172	R238	G301	A366	W428	G51
H114	Y113	A173	I239	V302	F367	L429	H114
R52	H114	Y174	A240	I303	E368	D430	R52
D53	L115	F175	E241	I303	V369	K431	D53
P54	H116	L176	F242	K306	G370	L432	P54
R55	A117	H179	R243	D307	P371	E433	R55
D56	L118	D119	K244	L308	L372	A434	D56
A57	D119	S309	L245	S309	A373	N435	A57
Q58	W120	K310	Y246	K310	S374	V436	Q58
H59	W121	A181	K247	W121	V375	K437	H59
F60	N122	V182	E248	V182	L376	A438	F60
T61	V123	L184	V249	L184	V377	D441	T61
Q62	N128	P185	R250	P185	Y379	D442	Q62
R63	A129	L197	F267	T341	Y379	D442	R63

E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
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E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536
E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E53				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 93.90Å 69.20Å 89.80° 102.90° 90.80°	Depositor
Resolution (Å)	8.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.3 (8.00-2.85)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, NI, FEL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	0/2014	1.43	12/2738 (0.4%)
1	C	0.84	0/2014	1.44	11/2738 (0.4%)
2	B	0.81	0/4251	1.45	37/5782 (0.6%)
2	D	0.81	0/4251	1.45	36/5782 (0.6%)
All	All	0.82	0/12530	1.45	96/17040 (0.6%)

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	190	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	B	414	ARG	NE-CZ-NH1	11.16	125.88	120.30
2	D	16	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	74	GLY	N-CA-C	10.34	138.94	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1961	0	1879	155	0
1	C	1961	0	1879	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4145	0	4073	362	1
2	D	4145	0	4073	487	1
3	A	16	0	0	2	0
3	C	16	0	0	3	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
All	All	12268	0	11904	1142	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

The worst 5 of 1142 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LEU:HD21	2:B:405:PHE:HZ	1.15	1.07
2:D:14:ILE:HG13	2:D:21:LEU:HD13	1.30	1.07
1:C:29:ASP:HB3	1:C:30:PRO:HD3	1.30	1.06
2:D:27:VAL:HG22	2:D:32:ILE:HA	1.38	1.02
1:A:29:ASP:HB3	1:A:30:PRO:HD3	1.41	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:ASP:OD2	2:D:31:LYS:NZ[1_565]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/264 (98%)	198 (76%)	42 (16%)	20 (8%)	1	1
1	C	260/264 (98%)	192 (74%)	43 (16%)	25 (10%)	0	0
2	B	528/536 (98%)	387 (73%)	94 (18%)	47 (9%)	0	0
2	D	528/536 (98%)	379 (72%)	97 (18%)	52 (10%)	0	0
All	All	1576/1600 (98%)	1156 (73%)	276 (18%)	144 (9%)	0	0

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	29	ASP
1	A	41	SER
1	A	79	GLY
2	B	35	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/211 (97%)	160 (78%)	45 (22%)	1	0
1	C	205/211 (97%)	161 (78%)	44 (22%)	1	0
2	B	431/441 (98%)	346 (80%)	85 (20%)	1	1
2	D	431/441 (98%)	330 (77%)	101 (23%)	0	0
All	All	1272/1304 (98%)	997 (78%)	275 (22%)	1	0

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	326	SER
2	D	365	GLU
2	D	478	GLU
2	B	342	LYS
2	B	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	HIS
2	D	72	HIS
1	C	124	ASN
1	C	235	GLN
2	D	172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	A	267	1	0,12,12	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
6	FEL	B	537	2	0,3,3	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
6	FEL	D	537	2	0,3,3	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	267	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	267	SF4	1	0
3	A	265	SF4	1	0
3	C	267	SF4	1	0
3	C	265	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.